Damping of Bloch oscillations in the Hubbard model

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Using nonequilibrium dynamical mean-field theory, we study the isolated Hubbard model in a static electric field in the limit of weak interactions. Linear response behavior is established at long times, but only if the interaction exceeds a critical value, below which the system exhibits an AC-type response with Bloch oscillations. The transition from AC to DC response is defined in terms of the universal long-time behavior of the system, which does not depend on the initial condition.

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In the absence of scattering of charge carriers in a metal, a static electric field results in undamped oscillations of the current, which are known as Bloch oscillations. The fate of these oscillations in the presence of strong inter-particle scattering is theoretically not well understood. Intuitively, one might expect them to get damped until a direct current (DC) is established at long times, which would then be given by the linear or nonlinear DC response of the system. In the following we demonstrate that this intuitive picture is not true in general for a closed system: For the Hubbard model, we show that an electric field induces a DC response only if the inter-particle interaction exceeds a critical value.

Bloch oscillations are most easily understood in a simple tight-binding model. For example, if a linear potential is added to a tight-binding chain with lattice spacing a, the single-particle spectrum changes from a continuous energy band to an infinite set of levels at integer multiples of the potential difference eaE between neighboring lattice sites (for a review, see Ref. [1]). The eigenstates of this so-called Wannier-Stark ladder are localized on a length $l \propto 1/E$, and beating oscillations at the Bloch frequency $\omega_B = eaE/\hbar$ arise from any linear superposition of those states. A direct experimental observation of Bloch oscillations in solids is hardly possible because extremely large fields are needed to make the period $2\pi/\omega_B$ short compared to typical scattering times. However, Bloch oscillations have been observed in semiconductor superlattices [2], and, within a well-controlled setup, using ultracold atomic gases in optical lattices [3].

Our initial question about the establishment of a DC regime becomes somehow trivial for a system that is coupled to a thermal bath. In this case one will always get a finite current at long times, although for large fields the magnitude of this current can exhibit an interesting dependence on the system-bath coupling [4]. A closed system, on the other hand, which is the appropriate representation for cold atoms in an optical lattice, cannot sustain a true steady state with nonzero current j in a constant field, because the energy $\mathcal{E}$ always changes at a rate $\dot{\mathcal{E}} = Ej$ (e.g., Ref. [5]). So the question arises how one can possibly define a transition from an oscillating to a direct current in such a system. As it turns out, the answer to this is already the key for understanding the nature of the transition itself: While the true steady current is zero, the system establishes a universal relation between its thermodynamic quantities and the current well before the final state is reached, and it is by means of this universal behavior that one can clearly separate a linear response-like DC regime from an alternating current (AC) regime, in which the system exhibits Bloch oscillations at long times.

In this paper we investigate the AC/DC transition within the half-filled Hubbard model,

$$H = \sum_{ij,\sigma=\uparrow,\downarrow} t_{ij}\, c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i \big(n_{i\uparrow} - \tfrac{1}{2}\big)\big(n_{i\downarrow} - \tfrac{1}{2}\big), \qquad (1)$$

which describes fermionic particles that can hop between the sites of a crystal lattice (with hopping amplitude t_{ij}) and interact with each other through a local Coulomb repulsion U. We will characterize the zero-current final state (which still feels the presence of both electric field and interaction), and demonstrate the existence of an AC/DC transition at an interaction $U > 0$. The results fit well into the picture established by a number of recent investigations on the topic. Exact diagonalization of the Bose Hubbard model shows a qualitative change of the many-body spectrum with increasing electric field [6], and for spinless fermions, Bloch oscillations are observed in an integrable version of the model, while a nonintegrable version shows overdamped behavior [5]. In the infinite-dimensional Falicov-Kimball model oscillations are damped [7], but the relaxation to the steady behavior is still not fully resolved there. Moreover, our findings link the damping of Bloch oscillations to the more general question how a closed system relaxes to a well-defined state. This question has been intensively discussed recently, in order to understand the thermalization of isolated many-body systems [8].

We solve the dynamics of the Hubbard model using the dynamical mean-field theory (DMFT) [9] in its nonequilibrium variant [10]. The electric field is treated in a gauge with zero scalar potential and time-dependent vector potential, $\boldsymbol{E} = -\frac{1}{c}\partial_t \boldsymbol{A}$. The latter enters the Hamiltonian (1) via a Peierls substitution, i.e, a time-dependent shift of the band energy $\epsilon(\boldsymbol{k}) \to \epsilon(\boldsymbol{k} - \boldsymbol{A})$. We

choose the field along the $(1, 1, \ldots, 1)$-direction in the infinite-dimensional hypercubic lattice with a Gaussian density of states $\rho(\epsilon) = e^{-\epsilon^2}/\sqrt{\pi}$. The unit of energy is given by the variance W of the density of states (the bandwidth), time is measured in units of $\hbar/W$, and the unit of the electric field is given by W/ea, where $-e$ is the electronic charge and a is the lattice spacing. The DMFT equations for this setup have been discussed in detail in Ref. [7], and our precise implementation is given in Ref. [11]. Because we are interested in the regime of weak coupling, we use iterated perturbation theory (IPT) [9] to solve the effective impurity problem of DMFT. For nonequilibrium, IPT can work very well for small U in spite of the fact that it is not conserving, but it breaks down rather abruptly if U is too large [12]. To validate our results, we have performed Monte Carlo simulations [13], which reproduce the AC/DC transition, but do not allow a systematic analysis of the long-time behavior.

If not stated otherwise, the results below show the time-evolution of the Hubbard model in a constant electric field, starting from the free Fermi sea at $t < 0$. Later we investigate various other initial states and switch-on procedures of the field in order to show that the conclusions of the paper do dot depend on them. To characterize the time-evolving state we compute the current $j(t) = \sum_{\boldsymbol{k}} \langle c^\dagger_{\boldsymbol{k}}(t) c_{\boldsymbol{k}}(t)\rangle \partial_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}}$ and the local spectral function (which is gauge-independent [14])

$$A(\omega, t) = -\frac{1}{\pi} \text{Im} \int_0^\infty ds \, G^{\mathrm{R}}(t+s, t) e^{i\omega s}, \qquad (2)$$

where $G^{\mathrm{R}}(t, t') = -i\Theta(t - t')\langle\{c(t), c^\dagger(t')\}_+\rangle$ is the retarded Green function. For $U = 0$, $A(\omega)$ resembles the Wannier-Stark ladder, $A(\omega) = \sum_m \delta(\omega - m\omega_B) w_m$, where the weights w_m are given by the amplitudes of the Wannier-Stark states which are localized at sites with a potential energy difference $m\hbar\omega_B$ [14].

Results — Figure 1a and b show the time-dependent current after an electric field $E = 0.5$ is suddenly turned on in the Hubbard model. With increasing interaction, the evolution of the current changes from damped Bloch oscillations (AC regime) to a monotonously decreasing current (DC regime), which is best visible on a logarithmic scale (Fig. 1b). For a quantitative characterization of the behavior we fit the data in the AC and DC regimes at long times with a damped oscillation $j(t) = A\cos(\omega t + \phi)\exp(-\lambda t)$ and an exponential decay $j(t) = A\exp(-\lambda t)$, respectively (Fig. 1c and d). The fits work well everywhere except close to the transition, where it apparently takes longer time until initial transients decay and a simple relaxation behavior is established (this will be discussed below).

In the AC regime, the decay rate $\lambda(U)$ increases linearly up to $U \approx E$, where it exhibits a kink and starts to rise more rapidly (Fig. 1c). This result can be understood within the Wannier-Stark picture: For the given geometry, the energy levels of the tight-binding model with

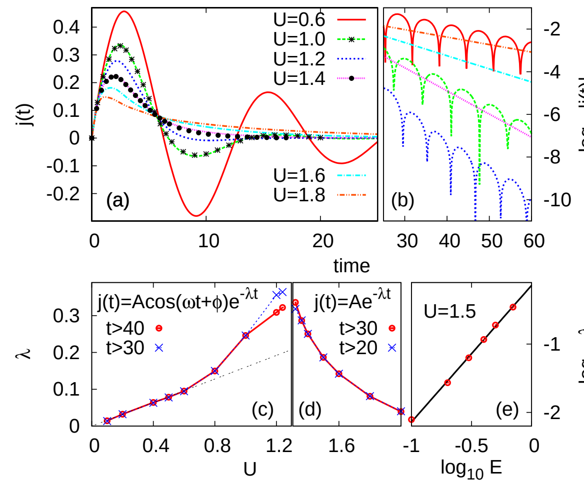

FIG. 1: (a) Current $j(t)$ for $E = 0.5$ and various values of U. For $t < 0$, the state is the noninteracting Fermi sea at $\beta = 10$. Lines: IPT, Symbols (for $U = 1.0$ and $U = 1.4$): QMC. (b) Same parameters as (a), on a logarithmic scale. (c,d) Damping rate $\lambda(U)$ for $E = 0.5$, obtained from fitting $j(t)$ with a damped oscillator (c) and an exponential decay (d), respectively. Each fit is computed for two time intervals to estimate the influence of the initial transients. (e) Damping rate $\lambda(E)$ for the DC regime ($U = 1.5$, exponential fit of $j(t)$). The line corresponds to $\lambda = \sigma_\infty/c_\infty E^2$, where $\sigma_\infty = 0.4172$ and $c_\infty = 0.122$ have been computed for $U = 1.5$ (see text).

linear potential are given by integer multiples $m\hbar\omega_B$ of the Bloch frequency, and each level is highly degenerate due to the translational invariance of the system transverse to the field. Any interaction $U \ll E$ will lift this degeneracy and lead to bands of width proportional to the matrix elements of the interaction operator in the manifold of Wannier-Stark states belonging to *one* energy. This splitting then leads to a dephasing of the oscillations at a rate proportional to U, and the kink can be associated with the fact that only for $U \gtrsim E$ scattering between Wannier Stark states with different m becomes effective. The argument is supported by the behavior of the spectral function (Fig. 2a). For $U \lesssim E$, we find that $A(\omega, t \to \infty)$ consists of well separated peaks with spacing E, whose weight is approximately given by the weight of the delta-peaks in the noninteracting spectrum of the Wannier Stark ladder. The gaps start to be filled for $U \gtrsim E$. Note that this crossover is not related to the transition between AC and DC regimes, which occurs only at larger values of U.

In the DC regime, the decay rate $\lambda(U)$ decreases with the interaction (Fig. 1d). A simple explanation of the exponential decay of the current in this regime is possible in the limit of small E: Because the system is not coupled to a reservoir, the total energy $\mathcal{E}$ increases a the rate $\dot{\mathcal{E}}(t) = Ej(t)$ [5]. The most simple assumption that one can make to account for this effect is that the system rapidly thermalizes, such that its state is a thermal

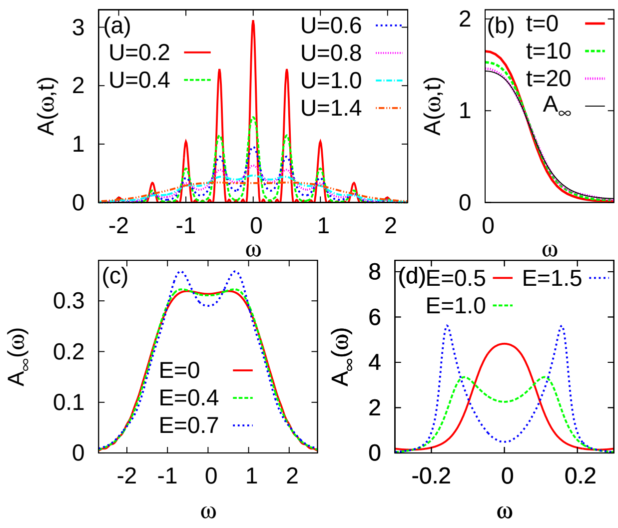

FIG. 2: (a) Retarded spectrum, Eq. (2), for the same parameters as in Fig. 1 ($E = 0.5$, $\beta = 10$). (b) $A(\omega, t)$ in the central frequency range for $U = 0.4$ and various times, compared to the final state spectrum $A_\infty(\omega; U, E)$. (c) The final state spectrum $A_\infty(\omega; U, E)$ in the DC regime ($U = 1.5$). (d) The central Wannier-Stark peak of $A_\infty(\omega; U, E)$ in the oscillating regime ($U = 0.4$), normalized to unit area.

equilibrium state with temperature $T_{\rm eff}(t)$ and energy $\mathcal{E}(t) = \mathrm{Tr}[e^{-H/T_{\rm eff}(t)}H]/Z$ at any given time t. (From a Boltzmann equation, the thermalization time would be expected to be $\propto U^{-2}$.) The current at small E is then given by the linear response value $j = \sigma_{\rm dc}E$. At long times, the system approaches $T_{\rm eff} \to \infty$, and both $\sigma_{\rm dc}$ and $\mathcal{E}$ are asymptotically given by the leading terms of their high-temperature expansion, $\sigma_{\rm dc} \sim \frac{\sigma_\infty}{T_{\rm eff}}$, $\mathcal{E} \sim -\frac{c_\infty}{T_{\rm eff}}$. Hence, energy and current obey a linear relation

$$j(t) \sim -E(\sigma_\infty/c_\infty)\,\mathcal{E}(t). \tag{3}$$

If this is inserted back into the exact relation $\dot{\mathcal{E}} = Ej(t)$, one finds that the current exhibits an exponential decay with rate $\lambda \sim \sigma_\infty/c_\infty E^2$ for $E \to 0$. As a numerical check in the present case we verify the linear relation between current and total energy at long times [Eq. (3)] by plotting $j(t)$ against $\mathcal{E}(t)$ in Fig. 3a. Also the E^2 dependence of λ is confirmed by our numerical results (Fig. 1e), where the coefficients c_∞ and σ_∞ are obtained by a solution of the DMFT equations in thermal equilibrium for $\beta \to 0$ (using IPT). Interestingly, an analogous argument holds for a nonintegrable model of spinless Fermions [5]. In contrast, rapid thermalization is impossible in the Mott insulating phase of the Hubbard model, such that a steady current can exist on rather long times [15].

Steady state — Both for the AC and the DC regimes we find that the system ultimately approaches a peculiar steady state which carries no current in spite of the electric field. To obtain an understanding of this state, we start from the limit of infinite temperature, which is the only equilibrium state with zero conductivity. In equilibrium, the Green functions $G^>(t,t') = -i\langle c(t)c^\dagger(t')\rangle$ and $G^<(t,t') = i\langle c^\dagger(t')c(t)\rangle$ are related by the fundamental relation $G^<(\omega) = -e^{\beta\omega}G^>(\omega)$, such that one has

$$G^<(t,t') = -G^>(t,t') = \tfrac{1}{2}[G^{\rm R}(t,t') - G^{\rm A}(t,t')] \tag{4}$$

at $\beta = 0$. This ansatz, which treats quantum mechanical creation and annihilation operators as commuting objects, can readily be used as the definition of a generalized infinite temperature state at nonzero E: It turns out that there is a unique steady-state solution $G^{\rm R}(t,t') \equiv g_\infty(t-t')$ of the DMFT equations which satisfies Eq. (4): If Eq. (4) is enforced, IPT diagrams for the retarded self-energy can be expressed in terms of retarded Green functions only, in contrast to a general state, where they depend on the occupation functions, $G^<(t,t')$ and $G^>(t,t')$. Hence, DMFT provides a closed set of equations for the the spectral (retarded) components of the Keldysh Green functions, which can be solved starting from the initial condition $G^{\rm R}(t,t) = -i$. In Fig. 2b we show that the spectral function (2) approaches $A_\infty(\omega) = -1/\pi \mathrm{Im} g_\infty(\omega)$ for long times, which provides evidence that the state of the Hubbard model in a field at $t \to \infty$ is indeed characterized by the ansatz (4). In spite of its strong excitation, this state is still strongly influenced by the field, both in the AC and DC regimes (Figs. 2c and d). In particular, the Hubbard bands are enhanced in the presence of the field. An explanation for this fact could be that for the given geometry hopping between sites on one equipotential surface is possible only by a second order process via a site at potential difference Eae, so the bandwidth is effectively reduced to W^2/Eae in the limit of strong fields.

The transition — The current traces in Fig. 1b show that the switch from oscillating to plain exponential decay in the long-time behavior defines a sharp transition line $U_{\rm ACDC}(E)$ in the E-U diagram (Fig. 3c). But how does this line depend on specifics of the system, such as initial conditions, or the way in which the field is turned on? Figure 3a and b show plots of the current against the total energy for one set of parameters in the AC and DC regime, respectively. By multiplication of $\mathcal{E}$ and j with a single scaling factor, all curves for fixed U and E collapse to a unique path in the long-time limit. This reveals the remarkable fact that the system follows a universal long-time behavior well before it reaches the final zero-current state discussed above. For small fields, this universal long-time behavior is precisely given by linear response theory [cf. Eq. (3)], but we can now see that the isolated Hubbard model actually follows this behavior only if the interaction exceeds the critical value $U_{\rm ACDC}$.

A universal long-time behavior naturally arises if the time-evolution for $t \to \infty$ can be described in terms of a linear equation for some reduced dynamical quantities $y(t)$. An example would be a Boltzmann equation, in

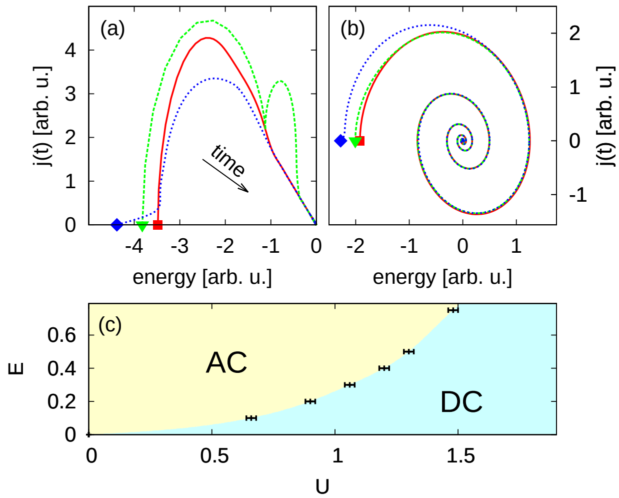

FIG. 3: (a) $j(t)$ plotted against the total energy $\mathcal{E}(t)$ at $E = 0.6$, $U = 1.8$ for various initial states: Sudden turn on of the field starting, from the noninteracting Fermi sea at $\beta = 9$ (square symbol), gradual turn on of the field, $E(t) = Et/t_0$, over a time-interval $t_0 = 10$ (diamond), and a sudden turn-on of the field starting from interacting thermal equilibrium at $\beta = 5$ and $U = 1.8$ (triangle). For each curve, j and $\mathcal{E}$ have been multiplied by a single scaling factor. (b) Same as (a), for $U = 0.6$ (c) $E - U$ phasediagram, showing regions where the long-time behavior is governed by oscillations (AC) or a direct current (DC).

which $y(t)$ are densities of relevant modes. If the equation is linearized close to a steady-state solution, the resulting linear equation has a number of exponentially decaying eigenmodes, of which the slowest survives at long times (with a single weight factor determined by the initial condition). A dynamical transition then occurs when the relaxation times for two such qualitatively different solutions cross as a control-parameter is changed. The fact that the decay rate $\lambda(U)$ increases towards the transition both in the AC and the DC regime is consistent with this interpretation (1c and d). Furthermore, close to the transition our data cannot be fit well with a simple relaxation law, since they look more like a superposition of oscillating and decaying terms which are hard to separate. However, the derivation of a linearized dynamical equation remains a unresolved issue for the present model. A starting point would be to linearize the exact time-evolution given by the Dyson equation around the final state given by the ansatz (4), but such a calculation seems rather involved due to the time-dependence of the gauge dependent $\boldsymbol{k}$-resolved Green function in this state.

Conclusion — In this paper we have studied the Hubbard model at weak U in a static electric field E. In spite of the fact that the system is not coupled to a thermal reservoir, a DC response is established at long times. However, this holds only if the interaction exceeds a critical value, below which the system exhibits an AC-type response with Bloch oscillations. This AC/DC transition is defined by the long-time behavior of the system, which does no longer depend on the initial condition. Furthermore, we have related the damping rate of the Bloch oscillations to the destruction of the Wannier-Stark ladder, and we have provided an understanding of the zero-current final state of the closed system in terms of a generalized infinite temperature state. Our results may be tested in experiments with ultracold atoms in optical lattices. Beyond this, we believe that a detailed understanding of the response of an isolated system is important in order to contrast studies of nonlinear transport in solid state bulk systems, where the precise form of the damping mechanism is often not known.

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